

Phase diagrams of the 2D $t - t' - U$ Hubbard model from an extended mean field method

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It is well-known from unrestricted Hartree-Fock computations that the 2D Hubbard model does not have homogeneous mean field states in significant regions of parameter space away from half filling. This is incompatible with standard mean field theory. We present a simple extension of the mean field method that avoids this problem. As in standard mean field theory, we restrict Hartree-Fock theory to simple translation invariant states describing antiferromagnetism (AF), ferromagnetism (F) and paramagnetism (P), but we use an improved method to implement the doping constraint allowing us to detect when a phase separated state is energetically preferred, e.g. AF and F coexisting at the same time. We find that such mixed phases occur in significant parts of the phase diagrams, making them much richer than the ones from standard mean field theory. Our results for the 2D $t - t' - U$ Hubbard model demonstrate the importance of band structure effects.

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I. INTRODUCTION AND MAIN RESULTS

Hubbard-type models in two dimensions have been frequently studied in the context of high temperature superconductivity and other strongly correlated systems.¹ Despite considerable efforts (for review see e.g. Ref. 2) there is still need for simple methods that can contribute to the understanding of the complex behavior of such models. In this paper we study an extension of mean field (MF) theory which allows for the possibility of phase separated states, in addition to the usual MF states. We calculate full phase diagrams for the 2D $t - t' - U$ Hubbard model which, to our knowledge, are not available in the literature by other methods.

MF theory offers several advantages compared to more complicated methods like unrestricted Hartree-Fock (HF) theory: It is easy to implement, not restricted to small system sizes, and can produce phase diagrams for Hubbard-type models with a limited computational effort. The disadvantage of *standard* MF theory is that it always predicts translation invariant states everywhere in the phase diagram, without giving any information about the stability with respect to fluctuations, or about the stability with respect to competing non-uniform states. In 2D Hubbard-type models these problems have severely restricted the usefulness of the MF approach,^{3,4} and the MF method is therefore not widely used. More correct methods indeed demonstrate that the qualitative features of the standard MF predictions are restricted to parts of the phase diagram, e.g., the antiferromagnetic (AF) phase at half filling. This suggests that the MF approach is unsatisfactory and motivates using more complicated methods. However, the more accurate theoretical methods tend to be computationally demanding and therefore restricted to very small system sizes.

In this paper we adopt and clarify the extended MF

method in Refs. 5,6 and use it to calculate phase diagrams of the 2D $t - t' - U$ Hubbard model. This method is designed to overcome the limitation of only producing uniform MF solutions, without increasing the computational effort. We use the standard mean field equations,^{3,4,7} but we extend them by a method allowing us to detect possible instabilities towards phase separation.⁶ The phase diagrams we thus obtain are much richer than the ones obtained with conventional MF theory and no longer in contradiction with unrestricted HF results. In particular, conventional MF theory for the 2D Hubbard model ($t' = 0$) predicts an AF phase in a finite doping regime around half filling (see Fig. 3 in Ref. 3) which is known to be qualitatively wrong. The phase diagram from the extended MF theory is shown in Fig. 1. It shows that the AF phase exists only strictly at half filling, and at finite doping close to half filling no simple translation invariant state is thermodynamically stable, in agreement with unrestricted HF theory.^{8,9,10,11} While our method does not account for fluctuations or details of states which are not translational invariant, it allows to detect frustration in the sense of incompatibility between MF states and the doping constraint. Such frustration suggests interesting physical behavior to be explored by more sophisticated methods. Our theory should be useful also for other cases where no other methods are available.

Our main results are the full phase diagrams for 2D $t - t' - U$ Hubbard model for $t' = 0$ and $t' = -0.35t$ in Figs. 1 and 2, respectively. They were obtained for a system size so large that they are practically identical with the thermodynamic limit. The phase diagrams are remarkably rich and very different from the corresponding results from standard MF theory: compare our Fig. 1 with Fig. 3 in Ref. 3 and our Fig. 2 with Fig. 1 in Ref. 4. Our results demonstrate that mixed phases are a typical feature of 2D Hubbard-type models: as one changes

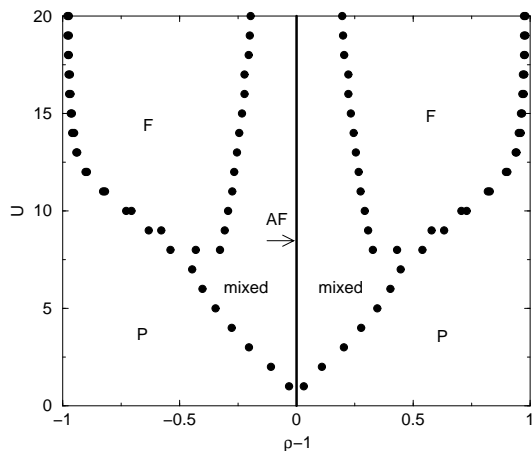


FIG. 1: Phase diagram of the 2D Hubbard model as a function of U and doping ρ for parameters $t = 1$ and $t' = 0$. We use Hartree-Fock theory restricted to ferromagnetic (F), antiferromagnetic (AF) and paramagnetic (P) states, and we find large mixed regimes where neither of these translational invariant states is thermodynamically stable. The results are for $L = 60$ and $\beta = 1000$ which is practically indistinguishable from the thermodynamic limit.

doping one never goes directly from one MF phase to another, but there seems always a finite doping regime with a mixed phase in between. It is also interesting to note that the qualitative features of the phase diagram are very sensitive to changes in the next-nearest-neighbor (NNN) hopping constant t' , in qualitative agreement with the unrestricted HF results.¹² In particular, while a pure AF phase is possible only at half filling for $t' = 0$, the AF phase can be doped by electrons, but not holes, for $t' < 0$ at larger values of U , in agreement with previous results obtained with a more complicated method.¹³

The plan of the rest of this paper is as follows. In the next section we explain and justify our method using physical arguments. Mathematical details can be found in Sec. III. Section IV contains our conclusion and a summary.

II. THE METHOD

We now explain our method, concentrating on the point where we deviate from standard MF theory. Precise mathematical formulas implementing this method will be given in the next section. As a representative example we discuss the computation of the phases by our method for the 2D Hubbard model with $U = 6$, and $t = 1$ and $t' = -0.16$ (see Eq. (6) below for the precise definitions). One reason for this choice is that it shows nicely several qualitative features which can occur in the phase diagram, another that these parameter values are of interest for high- T_c compounds.¹⁴

MF theory for the Hubbard model is obtained by re-

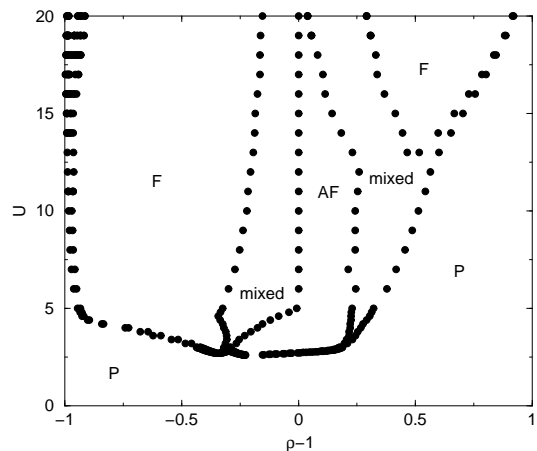


FIG. 2: Phase diagram of the 2D Hubbard model as a function of U and doping ρ for parameters $t = 1$, $t' = -0.35$, $L = 60$ and $\beta = 1000$, computed as Fig. 1. For large U and ρ close to zero it becomes numerically difficult to distinguish between the F and P phase, which is the reason for the fuzzy phase boundaries in this region of the phase diagram.

stricting HF theory to translational invariant states describing antiferromagnetism (AF), ferromagnetism (F) and paramagnetism (P).^{3,7} It would be straightforward to generalize this and also allow for charge-density waves, ferrimagnetism etc. One thus starts with three variational states which all are Slater determinants¹⁵ built of one-particle wave functions which are eigenstates of a mean field Hamiltonian where the Hubbard interaction is replaced by external field terms,

$$|\text{Slater}\rangle = |X\rangle, \quad X = \text{AF, F or P}. \quad (1)$$

These fields include the the fermions density ρ and the magnetization which is staggered for AF, constant for F, and zero for P, and they are determined by the usual Hartree-Fock equations. It is important to note that the fermion density is fixed in the standard Slater states, but we use a generalization of Slater's variational principle to Gibbs states allowing for finite temperature and where the fermion density is varied by changing a chemical potential μ (grand canonical ensemble).^{6,16,17} We now compute the Hartree-Fock ground state free energy per site, \mathcal{F}_X , for each of these states $X = \text{AF, F and P}$, as a function of μ .

Figure 3 gives the result for our example. At fixed value of μ , the mean field ground state is determined by the minimum,

$$\mathcal{F}_{\min} = \min_{X=\text{AF,F,P}} \mathcal{F}_X. \quad (2)$$

It is now important to note that the fermion density can be computed as derivative of the free energy as follows,

$$\rho - 1 = -\frac{\partial \mathcal{F}_{\min}}{\partial \mu}; \quad (3)$$

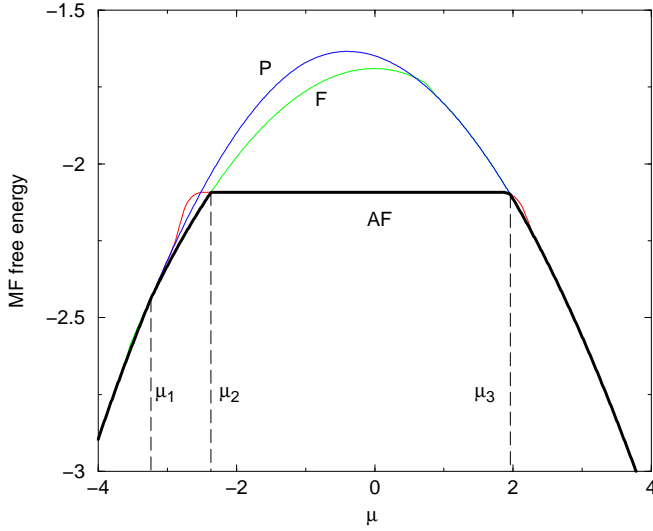


FIG. 3: Mean field free energy \mathcal{F}_X of the 2D Hubbard model with $t = 1$, $t' = -0.16$, $U = 6$, $L = 60$ and $\beta = 1000$ as a function of the chemical potential μ . Shown are the curves for $X = \text{AF}$, F and P (thin lines) and the absolute minimum \mathcal{F}_{\min} (thick line). The dashed lines indicate the particular values μ_i , $i = 1, 2, 3$, of μ where the phases change. At these values the derivative of \mathcal{F}_{\min} has discontinuities, and this leads to doping regimes with mixed phases; see Fig. 4.

we use conventions such that particle-hole symmetry is manifest, $\rho - 1 \rightarrow 1 - \rho$ corresponds to $\mu \rightarrow -\mu$ and $t' \rightarrow -t'$. From Figs. 3 and 4 it is obvious that this function $\rho - 1$ is, in general, only piecewise continuous, and it has jumps at the particular values of μ where the minimum free energy curve changes, for example, from the AF to the F curve at the value $\mu = \mu_2$. The physical interpretation of this is as follows. We start at $\mu = 0$ where we obviously have the AF ground state and half-filling, $\rho - 1 = 0$. As we decrease μ , $\rho - 1$ remains zero since \mathcal{F}_{AF} does not change. This is due to the AF gap: as long as μ remains in the gap the fermion density cannot change. For large enough μ values the AF band edge is reached and the slope of \mathcal{F}_{AF} starts to decrease. However, before this can happen the F free energy has become lower and taken over: as one decreases μ the F free energy decreases, and at a value $\mu = \mu_2$ the two curves cross, $\mathcal{F}_{\text{AF}} = \mathcal{F}_{\text{F}}$ at $\mu = \mu_2$. At this point we go from the AF to the F phase. Since the fermion densities $\rho_X(\mu_2) - 1 = -\partial\mathcal{F}_X/\partial\mu|_{\mu=\mu_2}$ for the states $X = \text{AF}$ and $X = \text{F}$ are different, it is impossible to get a density value in between with either state. There is, however, a possibility to realize such a fermion density with the following state *exactly* at $\mu = \mu_2$,

$$|\text{mixed}\rangle = w|\text{AF}\rangle + (1 - w)|\text{F}\rangle, \quad (4)$$

with the relative weight w determined by the density as follows,

$$\rho = w\rho_{\text{AF}}(\mu_2) + (1 - w)\rho_{\text{F}}(\mu_2), \quad 0 < w < 1. \quad (5)$$

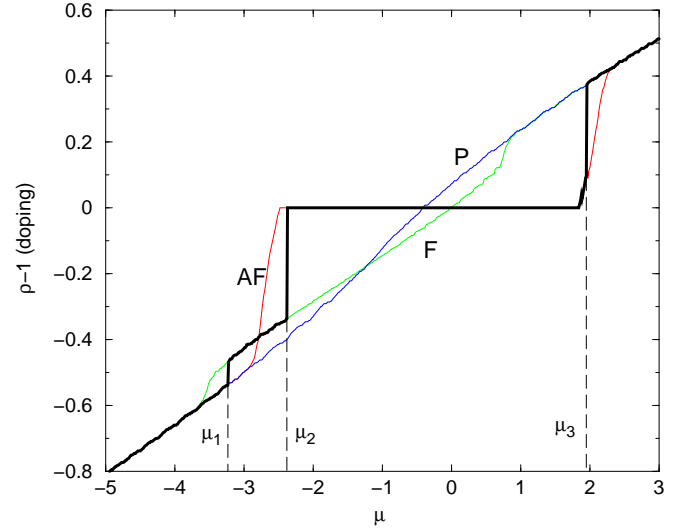


FIG. 4: Doping $\rho - 1$ of the 2D Hubbard model as a function of the chemical potential μ . The parameters are as in Fig 3 ($t = 1$, $t' = -0.16$, $U = 6$, $L = 60$ and $\beta = 1000$). The curves are the derivatives of the corresponding ones in Fig. 3. The thick line determines the mean-field phase diagram, with the discontinuities at $\mu = \mu_i$, $i = 1, 2, 3$ determining doping regions where no pure phase F, AF or P is thermodynamically stable. The wiggles of the curves are due to finite size effects which, however, have no effect on the phase boundaries (this is demonstrated in the inset of Fig. 5).

We now discuss the interpretation of this mixed solution. One possibility is that the system has phase separated and split up into AF and F regions.¹⁸ Of course, the spatial structure of the actual state is not available in the MF description by the mixed state, but it can in principle be calculated using unrestricted HF. However, since the bulk free energy dominates over the interfacial free energies in the thermodynamic limit, the mixed state gives an accurate description of the thermodynamics. We stress that the appearance of such a mixed state does *not* necessarily mean phase separation. The effect of the phase boundaries and other possible states have been excluded in our approximation. To know the actual state in the mixed regions thus is beyond our calculation and can be decided only by doing more work, e.g., using unrestricted HF taking into account more complicated states. Nevertheless, the *occurrence of such a mixed states proves that no simple translational invariant state of the kind assumed in our MF ansatz is thermodynamically stable*. The mixed regions of the phase diagram are of particular interest since there the free energy is degenerate and thus the details of the solution can be strongly affected by fluctuations, phase boundaries, or details neglected in the model.

It is important to note that there are two further jumps of ρ and two further corresponding mixed phases: one at $\mu = \mu_1$ with F coexisting with P, and another at $\mu = \mu_3$ with AF and P coexisting. It is also interesting to note

that, while for $t' = 0$ the mean field free energies are invariant under the electron-hole transformation $\mu \rightarrow -\mu$, the finite value of $t' = -0.16$ here leads to a qualitative difference between hole doping ($\mu < 0$) and electron doping ($\mu > 0$). As seen in Fig. 3, the F state can compete with the AF state only for $\mu < 0$, and this implies that it is possible to dope the AF state by electrons but not by holes.

We thus see that, even though we restricted Hartree-Fock theory to simple translation invariant states as in Eq. (1), our way of treating the doping constraint has implicitly also included the possibility of having a mixed state as in Eq. (4) as groundstate, and we find that such a mixed state indeed occurs in a significant part of the doping regime.

We stress that our method to determine the phase boundary does not increase the computational effort of mean field theory, and it is easy to do the computations also for large system sizes. Most of our computations were done for a $L \times L$ lattice with $L = 60$. While at this values of L some finite size effects are still visible in the relation between doping ρ and the chemical potential μ (see Fig. 4), the inset in Fig. 5 demonstrates that resulting phase boundaries are practically identical with the ones in the thermodynamic limit. We also checked that the value $\beta = 1000$ we used for the inverse temperature practically gives the zero temperature phase boundaries.

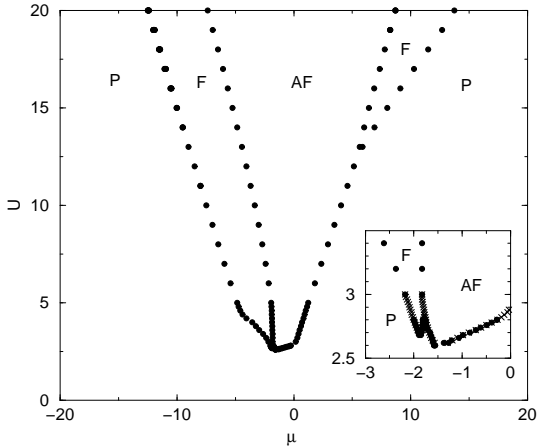


FIG. 5: Phases of the 2D Hubbard model as a function of the chemical potential for the same parameters as in Fig. 2 ($t = 1$, $t' = -0.35$, $\beta = 1000$, $L = 60$). Inset: Blowup of the region around the minimum of the phase lines in the main figure, showing interesting fine structure in the phase diagram. Also shown is the result from a calculation for system size $L = 120$ (crosses). The coincidence between results for two different system sizes demonstrate that $L = 60$ is practically already in the thermodynamic limit.

III. FORMALISM

We now give the formal implementation of our method. We start by fixing our notation. We consider the 2D Hubbard model defined by the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \alpha} c_{i,\alpha}^\dagger c_{j,\alpha} - t' \sum_{\langle\langle i,j \rangle\rangle, \alpha} c_{i,\alpha}^\dagger c_{j,\alpha} + \text{H.c.} - \mu \sum_{i,\alpha} c_{i,\alpha}^\dagger c_{i,\alpha} + U \sum_i (n_{i,\uparrow} - \frac{1}{2})(n_{i,\downarrow} - \frac{1}{2}) \quad (6)$$

with the on-site repulsion $U > 0$ and the hopping amplitudes $t > 0$ and t' between the nearest neighbor sites $\langle i, j \rangle$ and next-nearest neighbor (NNN) sites $\langle\langle i, j \rangle\rangle$ on a square lattice with L^2 sites, respectively; the fermion operators $c_{i,\alpha}^{(\dagger)}$ are parameterized by the spin variable $\alpha = \uparrow, \downarrow$ and lattice sites $i = (i_x, i_y)$ where $i_{x,y} = 1, 2, \dots, L$, and $n_{i,\alpha} = c_{i,\alpha}^\dagger c_{i,\alpha}$ are number operators, as usual. The fermion density is

$$\rho = \frac{1}{L^2} \sum_{i,\alpha} \langle n_{i,\alpha} \rangle \quad (7)$$

with $\langle \cdot \rangle$ the ground state expectation value to be specified below.

We recall that unrestricted Hartree-Fock (HF) theory is formally obtained by introducing

$$q_i = \langle n_i \rangle, \quad \mathbf{m}_i = \langle \mathbf{s}_i \rangle \quad (8)$$

and replacing the Hubbard interaction by external field terms as follows,

$$n_{i,\uparrow} n_{i,\downarrow} \rightarrow \frac{1}{4}(\mathbf{m}_i^2 - \rho_i^2) + \frac{1}{2}(q_i n_i - \mathbf{m}_i \cdot \mathbf{s}_i),$$

where $\frac{1}{2}U\mathbf{m}_i$ and $\frac{1}{2}Uq_i$ are mean fields coupling to the fermion spin $\mathbf{s}_i = \sum_{\alpha,\alpha'} c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\alpha'} c_{i,\alpha'}$ and (local) density $n_i = \sum_{\alpha} c_{i,\alpha}^\dagger c_{i,\alpha}$, respectively; $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the usual Pauli spin matrices. This replacement leads to a Hamiltonian describing non-interacting fermions in external fields, $H \rightarrow H_{HF}$ with

$$H_{HF} = \sum_i \frac{U}{4}(\mathbf{m}_i^2 - q_i^2) + \sum_{i,j,\alpha,\alpha'} c_{i,\alpha}^\dagger h_{i,\alpha,j,\alpha'} c_{j,\alpha'} \quad (9)$$

where

$$h_{i,\alpha,j,\alpha'} = -t_{ij}\delta_{\alpha\alpha'} + \delta_{ij} \left(\frac{1}{2}U[\mathbf{m}_i \cdot \boldsymbol{\sigma}_{\alpha\alpha'} + (q_i - 1)\delta_{\alpha\alpha'}] - \mu\delta_{\alpha\alpha'} \right) \quad (10)$$

is a self-adjoint $2L^2 \times 2L^2$ -matrix which can be interpreted as a one-particle Hamiltonian. One now interprets $\langle \cdot \rangle$ in Eq. (8) as the expectation value in the ground state of H_{HF} in Eqs. (9,10). This yields the HF equations allowing to self-consistently compute q_i and \mathbf{m}_i (see e.g. Sec. II in Ref. 11).

We now observe that these HF equations can also be obtained as saddle point equations $\partial\mathcal{F}/\partial\mathbf{m}_i = \partial\mathcal{F}/\partial\rho_i = 0$ from the free energy function

$$\mathcal{F} = -\frac{1}{\beta L^2} \log \mathcal{Z} \quad (11)$$

where

$$\mathcal{Z} = \text{Tr}(e^{-\beta H_{\text{HF}}}) \quad (12)$$

is the partition function defined by a trace over the fermion Hilbert space, and β is the inverse temperature. A straightforward computation yields

$$\mathcal{F} = \frac{U}{4L^2} \sum_i (\mathbf{m}_i^2 - \rho_i^2) - \frac{1}{L^2} \sum_{\ell=1}^{2L^2} \log \cosh \frac{\beta E_\ell}{2}, \quad (13)$$

with E_ℓ the eigenvalues of the one-particle Hamiltonian $h = (h_{i,\alpha,j,\alpha'})$ in Eq. (10).⁶

The physical solution of the HF equations are such that

$$\mathcal{F}_{\min} \equiv \min_{\mathbf{m}_i} \max_{q_i} \mathcal{F}(\mathbf{m}_i, q_i); \quad (14)$$

see Ref. 17 for a mathematical proof or Ref. 6 for a derivation using functional integrals. The corresponding fermion density is then given by Eq. (3). We stress that Eq. (14), while *implying* standard HF theory, is not equivalent to it: the standard HF equations can have several solutions, but Eq. (14) provides a simple method to solve HF equations so as to avoid the unphysical solutions: first maximize \mathcal{F} with respect to the q_i , and then minimize with respect to the \mathbf{m}_i . In case we restrict HF theory by making a simplifying ansatz for the mean fields q_i and \mathbf{m}_i as below, it can happen that one finds several HF solutions at a fixed value of μ . In this case one must take the solution minimizing \mathcal{F} .

Mean field theory is obtained from HF by restricting to mean fields which are invariant under translations by two sites. For the different states discussed in this paper one further simplifies to

$$\begin{aligned} \text{AF :} \quad & q_i = q, \quad \mathbf{m}_i = m_{\text{AF}}(-1)^{i_x+i_y} \mathbf{e}_z \\ \text{F :} \quad & q_i = q, \quad \mathbf{m}_i = m_{\text{F}} \mathbf{e}_z \\ \text{P :} \quad & q_i = q, \quad \mathbf{m}_i = \mathbf{0} \end{aligned} \quad (15)$$

where \mathbf{e}_z is the unit vector in z -direction. With this restrictions it is easy to compute the eigenvalues E_ℓ by Fourier transform. One obtains

$$\begin{aligned} \text{AF :} \quad & E_{\mathbf{k},\pm} = \frac{1}{2} [\epsilon(\mathbf{k}) + \epsilon(\mathbf{k} + \mathbf{Q})] + U(q-1) - \mu \pm \\ & \pm \sqrt{[\epsilon(\mathbf{k}) - \epsilon(\mathbf{k} + \mathbf{Q})]^2 + (Um_{\text{AF}})^2} \\ \text{F :} \quad & E_{\mathbf{k},\pm} = \epsilon(\mathbf{k}) + U(q-1 \pm m_{\text{F}}) - \mu \\ \text{P :} \quad & E_{\mathbf{k},\pm} = \epsilon(\mathbf{k}) + U(q-1) - \mu \end{aligned} \quad (16)$$

where the quantum numbers labeling the eigenvalues are $\ell \equiv (\mathbf{k}, \epsilon)$ with $\epsilon = \pm$ a band index and $\mathbf{k} = (k_x, k_y)$

with $k_{x,y} = (2\pi/L) \times \text{integer momenta}$ restricted to the Brillouin zone $-\pi \leq k_{x,y} \leq \pi$; $\mathbf{Q} = (\pi, \pi)$ is the AF vector, and

$$\epsilon(\mathbf{k}) = -2t[\cos(k_x) + \cos(k_y)] - 4t' \cos(k_x) \cos(k_y) \quad (17)$$

is the usual tight binding band relation. Thus the mean field free energy becomes

$$\mathcal{F}_X = \frac{U}{4} (m_X^2 - q^2) - \frac{1}{L^2} \sum_{\mathbf{k}, \epsilon=\pm} \cosh \frac{\beta}{2} E_{\mathbf{k},\epsilon} \quad (18)$$

for $X = \text{AF, F and P}$ ($m_{\text{P}} = 0$), where the \mathbf{k} -sum becomes an integral in the thermodynamic limit $L \rightarrow \infty$. The standard mean field equations (see e.g. Sec. II in Ref. 4) are obtained from this from differentiation, $\partial\mathcal{F}_X/\partial q = \partial\mathcal{F}_X/\partial m_X = 0$. Note that $q = \rho_X$ (fermion density at fixed μ in the X -state) but, as explained in Sec. II, the relation of ρ_X to the system density ρ is somewhat subtle.

IV. CONCLUSIONS AND DISCUSSION

In conclusion, we have presented a simple generalization of standard mean field theory, including the possibility of phase separated mean field states. We have presented results for the phase diagram of the 2D $t - t' - U$ Hubbard model, including values of parameters suggested by the high- T_c materials. We find that the NNN hopping t' significantly alters the solution. The resulting rich and nontrivial phase diagrams show significant qualitative differences between electron and hole doping. Moreover, a finite t' suppresses order in the weak coupling regime, but can have the opposite effect at strong coupling; see Figs. 2 and 5. Thus the results presented here are much richer than those obtained by standard MF theory.^{3,4} The correctness of our method is justified by mathematical rigorous results.¹⁷

We stress that the method presented here does not necessarily produce accurate solutions to the problem, as is often the case with mean field theory. Nevertheless the method provides a useful starting point for estimating the structure of the phase diagram, providing cheap guidance for more accurate but costly calculation methods towards interesting regimes in the phase diagram.

The simple theory presented here can be straightforwardly generalized to a number of interesting cases, including more general mean field states like ferrimagnetism or stripes, and to more complicated models with additional interaction terms or more bands, etc.

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